# Least Squares Methods for Equidistant Tree Reconstruction

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**Abstract**

UPGMA is a heuristic method identifying the least squares equidistant phylogenetic tree given empirical distance data among $n$ taxa. We study this classic algorithm using the geometry of the space of all equidistant trees with $n$ leaves, also known as the Bergman complex of the graphical matroid for the complete graph $K_n$. We show that UPGMA performs an orthogonal projection of the data onto a maximal cell of the Bergman complex. We also show that the equidistant tree with the least (Euclidean) distance from the data is obtained from such an orthogonal projection, but not necessarily given by UPGMA. Using this geometric information we give an extension of the UPGMA algorithm. We also present a branch and bound method for finding the best equidistant tree. Finally, we prove that there are distance data among $n$ taxa which project to at least $(n-1)!$ equidistant trees.

## 1 Introduction

We study the problem of finding the least squares equidistant tree given distance data between the elements of a finite set $X$ of cardinality $n$. The set $X$ is often a collection of taxa in biological applications. In this paper we will usually let $X = \{1, 2, \ldots, n\}$ unless otherwise stated. The distance data is given by a *dissimilarity map*, a real-valued function $d : \binom{[n]}{2} \longrightarrow \mathbb{R}$ defined for pairs $(i, j)$ where $1 \le i < j \le n$. We will represent a dissimilarity map by the edge weights of the complete graph $K_n$ of $n$ vertices where the weight of the edge $(i, j)$ in $K_n$ is $d(i, j)$.

Let $T$ be a (not necessarily binary) weighted tree with a root $r$ and $n$ leaves. The weight of each edge $e \in T$ will be denoted by $w_T(e)$, and we will omit the

subscript when the context makes it clear which tree we refer to. Given such a tree we get a distance function $x(a,b) = \sum_{e \in P_{a,b}} w_T(e)$ where $P_{a,b}$ is the unique path between the nodes $a$ and $b$ in $T$. A tree is called *equidistant* if $x(i,r)$ is the same real number for each leaf $i = 1, \ldots, n$. Note that we label the leaves of $T$ by $X$. A tree is equidistant if and only if for each distinct $i, j, k \in X$, the set of distances $\{x(i,j), x(i,k), x(j,k)\}$ achieves its maximum at least twice [4, 19, 22]. These are the *ultrametric* conditions.

With these definitions we can present the main problem of this paper: given a dissimilarity map $d$ on $X = \{1, \ldots, n\}$ find an equidistant tree $T$ on $n$ leaves such that

$$\sum_{1 \le i < j \le n} (d(i,j) - x(i,j))^2$$

is minimized. It is known that this problem (as well as the unrooted nonequidistant version) is NP complete [13, 14, 15].

The problem of tree construction arises in biology, where the goal is to describe the evolutionary history of species or genes. An equidistant tree approximates the true evolutionary history. The distances between species may be measured using several different methods, but currently distances are most often determined by comparison of aligned nucleic acid or amino acid sequences. One of several models of evolution is used to correct for the possibility of multiple substitutions at any one site [10]. When the rate of nucleotide or amino acid substitution was constant over the time period being considered, the ultrametric conditions are close to being satisfied. This condition is the *molecular clock hypothesis,* and if it holds a least squares equidistant tree could be used to fit the distance data. Least squares methods for tree construction are attractive because they are statistically consistent: the correct tree will be identified in the limit as the length of the sequences grows [9, 10]. In many cases the molecular clock hypothesis is not satisfied, and trees that are additive but not equidistant are preferred.
The Unweighted Pair Group Method with Arithmetic Means (UPGMA) algorithm is a heuristic method for finding the least squares equidistant tree [10]. The UPGMA algorithm has polynomial time complexity, and works well on data which shows clock-like behavior. Even if the molecular clock holds, however, the UPGMA algorithm may return a tree that is not the best by the least squares criterion, as shown in Example 2.5 below. The unweighted least squares approach was first suggested by Cavalli-Sforza and Edwards [5]. Other, related algorithms include the pioneering weighted least squares algorithm of Fitch and Margoliash [11], the transformed distances method [8], and neighbor-joining [18]. Neighbor-joining and recent variants BIONJ

[12] and weighbor [3] are not strictly least squares algorithms. Of all these UPGMA is particularly interesting here, as it arises naturally as a greedy algorithm from the approach described below. When the Euclidean metric is replaced by $\ell_\infty$ metric, a fast exact algorithm is known [6]. A conceptual explanation of this algorithm is given in [1].

Here we first describe UPGMA. We will present a version that outputs the combinatorial description of $T$ and $x(i,j)$ for each pair of leaves $i$ and $j$. It is well-known how to compute the edge weights $w_T(e)$ from these data. Recall that we represent the dissimilarity map $d$ as the edge weights of $K_n$.

**Algorithm 1.1.** UPGMA
**Input** : Complete graph $K_n$ with edge weights $d(i,j)$.
**Output**: An equidistant tree $T$ with leaves $X = \{1,\ldots,n\}$ and $x(i,j)$ for each $i,j \in X$.

$G := K_n$.
$V(T) := X$, $E(T) := \emptyset$, and $S(T) := X$.
**repeat**

$$minave := \min_{v,w \in V(G)} \frac{1}{C(v,w)} \sum_{(i,j) \in E(v,w)} d(i,j)$$

where $E(v,w)$ is the set of edges between the nodes $v$ and $w$ in $G$, and $C(v,w) = |E(v,w)|$.
Let $s$ and $t$ in $V(G)$ be the vertices for which the minimum above is attained.
Set $x(i,j) := minave$ for all $(i,j) \in E(s,t)$.
$G := G/\{s,t\}$, obtained by contracting the vertices $s$ and $t$ into a single vertex $st := s \cup t$.
$S(T) := S(T) \setminus \{s,t\} \cup \{st\}$.
$V(T) := V(T) \cup \{st\}$, $E(T) := E(T) \cup \{st, s\} \cup \{st, t\}$.
**until** $G$ has one vertex

Output $T$ and $x(i,j)$ $1 \le i < j \le n$. □

In Section 2 we describe the Bergman complex $\mathcal{B}_n$, namely, the space of all equidistant trees on $n$ leaves. We prove that Algorithm 1.1 performs an orthogonal projection (with respect to the usual Euclidean inner product) onto a maximal cell of $\mathcal{B}_n$. We give an example where already for $n = 4$ the UPGMA tree can be arbitrarily worse than the best equidistant tree. In

Section 3 we prove that the best equidistant tree is obtained by an orthogonal projection onto some maximal cone of $\mathcal{B}_n$. Motivated by this result we introduce a polyhedral subdivision of the data space $\mathbb{R}^{\binom{n}{2}}$ where each maximal cell consists of data vectors which project onto the same set of maximal Bergman cells. We show that the collection of such Bergman cells could be disconnected (in a sense made precise in Section 3). In fact, there are data vectors in $\mathbb{R}^{\binom{n}{2}}$ which project onto at least $(n-1)!$ Bergman cells, and we conjecture that this is the most number of projections one can obtain. Furthermore, we classify all data vectors in $\mathbb{R}^6$ which project onto six Bergman cells. In Section 4 we introduce two algorithms based on our results in Section 3. One of them is an extension of UPGMA that finds at least as good a tree as the UPGMA tree. The other one finds the best equidistant tree using a branch and bound approach. Section 5 concludes with an example where we analyze data for the timing and the sequence of the appearance of mammalian orders.

# 2 The Bergman complex and UPGMA

It is not difficult to show that Algorithm 1.1 indeed returns an equidistant tree using the ultrametric characterization of equidistant trees. Here we will describe the space of all vectors $x = (x(i,j) : 1 \leq i < j \leq n) \in \mathbb{R}^{\binom{n}{2}}$ which come from weighted equidistant trees with $n$ leaves, and from this description it will follow that the UPGMA produces an equidistant tree. Ardila and Klivans [2] described this space as a special case of the tropicalization of a linear variety, or more combinatorially, as the *Bergman complex* $\mathcal{B}_n$ of the graphical matroid of $K_n$. This description shows that $\mathcal{B}_n \subset \mathbb{R}^{\binom{n}{2}}$ is a polyhedral complex of dimension $n-1$: its maximal cones are polyhedral cones of dimension $n-1$, and any collection of them intersects in a face that belongs to each cone in the collection.

We first describe a different polyhedral complex $\mathcal{F}_n$ of dimension $n-1$ that is a refinement of $\mathcal{B}_n$, i.e. the maximal cones of $\mathcal{F}_n$ further subdivide the ones in $\mathcal{B}_n$. Given a graph $G$ on $m \leq n$ vertices which are labeled by disjoint subsets of $[n]$, and two vertices labeled $s$ and $t$ we obtain $G/\{s,t\}$, the *contraction* of $G$ on $\{s,t\}$, where

$$V(G/\{s,t\}) = V(G) \setminus \{s,t\} \bigcup \{st\} \quad \text{and} \quad E(G/\{s,t\}) = E(G) \setminus E(s,t)$$

where $E(s,t)$ is the set of edges between the vertices $s$ and $t$. We label the vertices $K_n$ with the singletons $\{1\}, \ldots, \{n\}$, and we call a graph $G$ obtained

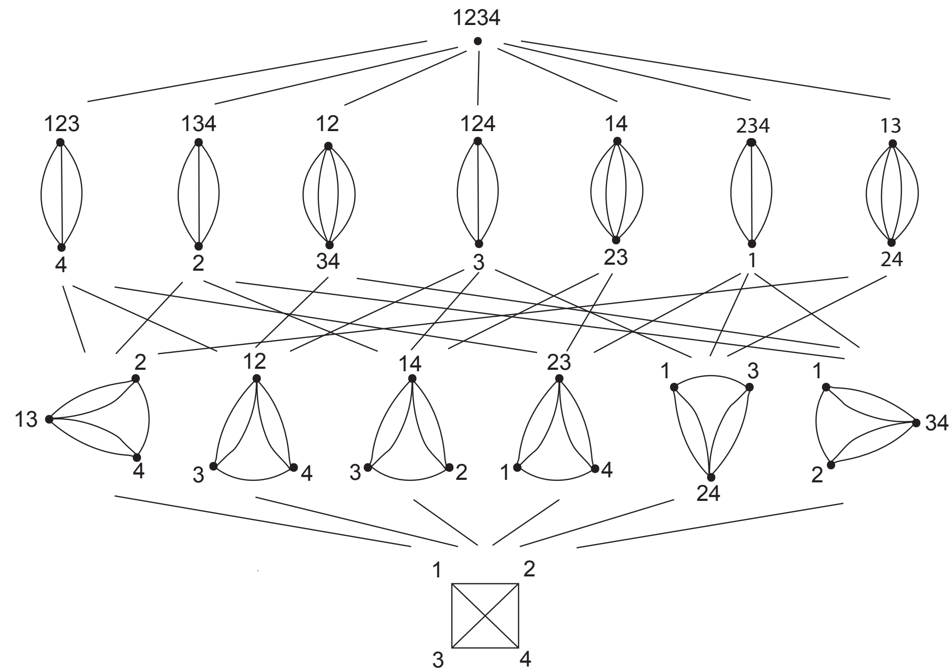


Figure 1: Lattice of contractions of $K_4$

by a sequence of contractions from $K_n$ a contraction of $K_n$. Contractions of $K_n$ form a lattice where $H \geq G$ if H can be obtained by a sequence of contractions from $G$. This lattice is isomorphic to the partition lattice $\Pi_n$ which is in turn isomorphic to the lattice of flats of $K_n$ ordered by inclusion: a flat of $K_n$ is the set of edges that are *not* present in a contraction of $K_n$. Figure 1 illustrates the lattice of contractions of $K_4$.
Now let $\mathcal{F} = \{\emptyset = F_0 \subset F_1 \subset F_2 \subset \cdots \subset F_{n-2} \subset F_{n-1} = \binom{[n]}{2}\}$ be a maximal chain of flats of $K_n$ obtained from $K_n$ by a sequence of $n-1$ contractions to $K_1$ with the vertex label $[n]$. Note that $F_i \setminus F_{i-1}$ is $E(s,t)$ for the corresponding contraction. We define a cone that is associated to $\mathcal{F}$ as

$$\begin{aligned} C_{\mathcal{F}} \quad = \quad & \Big\{(x(i,j)) \in \mathbb{R}^{\binom{n}{2}} : \\ & \{x(k,l) = x(s,t) : (k,l),(s,t) \in F_1 \setminus F_0\} \quad \leq \\ & \{x(k,l) = x(s,t) : (k,l),(s,t) \in F_2 \setminus F_1\} \quad \leq \cdots \leq \\ & \{x(k,l) = x(s,t) : (k,l),(s,t) \in F_{n-1} \setminus F_{n-2}\}\Big\}. \end{aligned}$$

The set of $C_{\mathcal{F}}$ as $\mathcal{F}$ ranges over all maximal chains in $\Pi_n$ is the maximal

cones of $\mathcal{F}_n$. As we mentioned above the maximal cones of the Bergman complex $\mathcal{B}_n$ are refined by the cones in $\mathcal{F}_n$. Indeed, two cones $C_{\mathcal{F}^1}$ and $C_{\mathcal{F}^2}$ belong to the same maximal cone in $\mathcal{B}_n$ if the chain of flats $\mathcal{F}^1$ and $\mathcal{F}^2$ differ exactly in one flat, say $F_i^1 \neq F_i^2$, and $(F_i^1 \setminus F_{i-1}^1) \cap (F_i^2 \setminus F_{i-1}^2) = \emptyset$.

**Example 2.1.** There are two types of cones corresponding to two types of flag of flats in $K_4$, namely,

$$\mathcal{F} = \{\emptyset \subset \{(1,2)\} \subset \{(1,2),(1,3),(2,3)\} \subset \binom{[4]}{2}\} \text{ and}$$

$$\mathcal{F}' = \{\emptyset \subset \{(1,2)\} \subset \{(1,2),(3,4)\} \subset \binom{[4]}{2}\}.$$

These go with two types of trees on four leaves: the comb and the fork in Figure 2. The corresponding maximal cones in $\mathcal{F}_4$ are:

$$C_{\mathcal{F}} = \Big\{(x(i,j)) \in \mathbb{R}^6 \,:\, x(1,2) \leq x(1,3) = x(2,3) \leq x(1,4) = x(2,4) = x(3,4)\Big\}$$

$$C_{\mathcal{F}'} = \Big\{(x(i,j)) \in \mathbb{R}^6 \,:\, x(1,2) \leq x(3,4) \leq x(1,3) = x(1,4) = x(2,3) = x(2,4)\Big\}$$

**Proposition 2.2.** *The UPGMA algorithm produces an equidistant tree.*

*Proof.* It is clear that this algorithm performs a sequence of contractions starting from $K_n$ and ending in $K_1$. At iteration $i$ of the repeat loop we let $F_i \setminus F_{i-1}$ to be $E(s,t)$ that has been identified. The algorithm sets $x(i,j) = x(k,l)$ for all $(i,j),(k,l) \in E(s,t)$. So we just need to show that $x(a,b) \leq x(c,d)$ for $(a,b) \in F_i \setminus F_{i-1}$ and $(c,d) \in F_{i+1} \setminus F_i$. We let the edges identified in the $(i+1)$st loop to be $E(v,w)$. There are two cases: either one of $v$ or $w$ is $s \cup t$ or not. In the second case

$$x(a,b) \;=\; \frac{1}{C(s,t)} \sum_{(i,j)\in E(s,t)} d(i,j) \quad \leq \quad \frac{1}{C(v,w)} \sum_{(i,j)\in E(v,w)} d(i,j) \;=\; x(c,d).$$

For the first case, without loss of generality we assume $v = s \cup t$ and

$$\frac{1}{C(s,t)} \sum_{(i,j)\in E(s,t)} d(i,j) \;\leq\; \frac{1}{C(s,w)} \sum_{(i,j)\in E(s,w)} d(i,j) \;\leq\; \frac{1}{C(t,w)} \sum_{(i,j)\in E(t,w)} d(i,j).$$

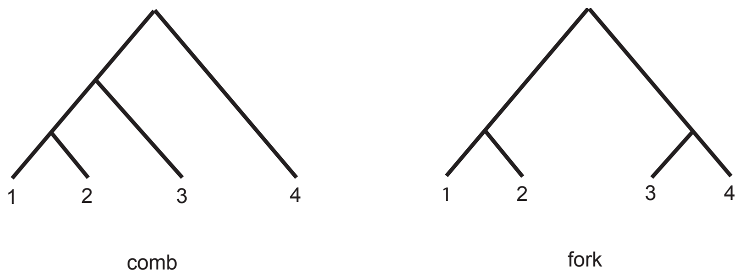


Figure 2: Comb and fork trees on four leaves

Now since $\frac{1}{C(v,w)} \sum_{(i,j) \in E(v,w)} d(i,j)$ is equal to

$$\frac{C(s,w)}{C(v,w)} \left( \frac{1}{C(s,w)} \sum_{(i,j) \in E(s,w)} d(i,j) \right) + \frac{C(t,w)}{C(v,w)} \left( \frac{1}{C(t,w)} \sum_{(i,j) \in E(t,w)} d(i,j) \right)$$

and $C(v,w) = C(s,w) + C(t,w)$ we get the desired inequality in this case as well. $\square$

In the rest of the paper, we will denote the cone in $\mathcal{F}_n$ which the UPGMA identifies as $C_{UPGMA}$.

**Proposition 2.3.** *If $(x(i,j))$ is the vector that the UPGMA outputs on the input of the vector $(d(i,j))$ then $(x(i,j))$ is the orthogonal projection of $(d(i,j))$ onto $C_{UPGMA}$.*

*Proof.* Let $\mathcal{F} = \{\emptyset = F_0 \subset F_1 \subset F_2 \subset \cdots \subset F_{n-2} \subset F_{n-1} = [n]\}$ be the chain of flats that define the cone $C_{UPGMA}$. Let $L_{UPGMA}$ be the smallest

subspace containing $C_{UPGMA}$. This subspace is defined by

$$\begin{aligned} L_{UPGMA} \;=\; & \Big\{ (x(i,j)) \in \mathbb{R}^{\binom{n}{2}} \;: \\ & x(k,l) = x(s,t) \;\forall\; (k,l),(s,t) \in F_1 \setminus F_0 \quad \text{and} \\ & x(k,l) = x(s,t) \;\forall\; (k,l),(s,t) \in F_2 \setminus F_1 \quad \text{and} \quad \cdots \\ & x(k,l) = x(s,t) \;\forall\; (k,l),(s,t) \in F_{n-1} \setminus F_{n-2} \Big\}, \end{aligned}$$

and it has an orthonormal basis consisting of the set of vectors

$$\Big\{ \frac{1}{\sqrt{|F_i \setminus F_{i-1}|}} \sum_{(s,t) \in F_i \setminus F_{i-1}} e(s,t) \quad : \quad i = 1, \ldots, n-1 \Big\}$$

where $e(s,t) \in \mathbb{R}^{\binom{n}{2}}$ is the standard unit vector corresponding to the edge $(s,t)$ of $K_n$. The linear projection formula with respect to this orthonormal basis implies that $x(v,w)$ coordinate of the projection of $(d(i,j))$ is equal to

$$\frac{1}{|F_k \setminus F_{k-1}|} \sum_{(i,j) \in F_k \setminus F_{k-1}} d(i,j)$$

with $(v,w) \in F_k \setminus F_{k-1}$. Note that if $(v,w)$ belongs to the contracted edges $E(s,t)$ during the UPGMA that produced $\mathcal{F}$, then $E(s,t) = F_k \setminus F_{k-1}$ and $C(s,t) = |F_k \setminus F_{k-1}|$, and therefore the projected vector $(x(i,j))$ is precisely the vector generated by UPGMA. Therefore this projected vector is not only in $L_{UPGMA}$ but also in $C_{UPGMA}$. This shows that UPGMA performs an orthogonal projection of $(d(i,j))$ onto $C_{UPGMA}$. $\square$

**Corollary 2.4.** *When $n = 3$ UPGMA produces the least squares tree.*

*Proof.* We assume that $d(1,2) \leq d(1,3) \leq d(2,3)$. The two fans $\mathcal{B}_3$ and $\mathcal{F}_3$ are identical with three cones described by the three chains of flats

$$\mathcal{F}_{12} = \{\emptyset \subset \{(1,2)\} \subset \binom{[3]}{2}\}, \; \mathcal{F}_{13} = \{\emptyset \subset \{(1,3)\} \subset \binom{[3]}{2}\}, \; \mathcal{F}_{23} = \{\emptyset \subset \{(2,3)\} \subset \binom{[3]}{2}\}.$$

UPGMA produces the tree in $C_{\mathcal{F}_{12}}$ where the leaves labeled with 1 and 2 form a cherry, and

$$x(1,2) = d(1,2) \quad \text{and} \quad x(1,3) = x(2,3) = (d(1,3) + d(2,3))/2.$$

The square distance of this tree to the data point is $(d(2,3) - d(1,3))^2/2$. We can orthogonally project the data point onto $L_{\mathcal{F}_{13}}$ and $L_{\mathcal{F}_{23}}$ to obtain

$x(1,3) = d(1,3)$, $x(1,2) = x(2,3) = (d(1,2) + d(2,3))/2$ and $x(2,3) = d(2,3)$, $x(1,2) = x(1,3) = (d(1,2) + d(1,3))/2$, respectively. The first projection is in $C_{\mathcal{F}_{13}}$ if and only if $d(1,3) \leq (d(1,2) + d(2,3))/2$, and the second projection is never in $C_{\mathcal{F}_{23}}$ unless $d(1,2) = d(1,3) = d(2,3)$. Theorem 3.4 implies that the best tree is either the UPGMA tree or the tree obtained from $C_{\mathcal{F}_{13}}$ if the projection falls into this cone. Since the square distance from the data point to this projection is $(d(2,3) - d(1,2))^2/2 \geq (d(2,3) - d(1,3))^2/2$ we get the result. $\square$

**Example 2.5.** When $n = 4$ UPGMA tree may be arbitrarily worse than the least squares tree. Let the data be $(d(i,j)) = (d(1,2), \ldots, d(3,4)) = (1, 2, 20, 10, 28 + \epsilon, 5)$. The UPGMA tree is obtained by contracting the edge $(1,2)$ and then $(3,4)$ in $K_4$. This gives us $(x(i,j)) = (x(1,2), \ldots, x(3,4)) = (1, 15 + \frac{1}{4}\epsilon, 15 + \frac{1}{4}\epsilon, 15 + \frac{1}{4}\epsilon, 15 + \frac{1}{4}\epsilon, 5)$, and the square distance from $(d(i,j))$ to $(x(i,j))$ is $388 + 31\epsilon + \frac{3}{4}\epsilon^2$. The data point can also be orthogonally projected onto the cone $C_{\mathcal{F}}$ where $\mathcal{F} = \{\emptyset \subset F_1 \subset F_2 \subset F_3 = \binom{[4]}{2}\}$ with $F_1 = \{(1,2)\}$, $F_2 \setminus F_1 = \{(1,3), (2,3)\}$, and $F_3 \setminus F_2 = \{(1,4), (2,4), (3,4)\}$. The resulting point is $(y(i,j)) = (1, 6, 6, \frac{53}{3} + \frac{1}{3}\epsilon, \frac{53}{3} + \frac{1}{3}\epsilon, \frac{53}{3} + \frac{1}{3}\epsilon)$, and the square distance from $(d(i,j))$ to $(y(i,j))$ is $\frac{914}{3} + \frac{214}{9}\epsilon + \frac{2}{3}\epsilon^2$. The first expression is greater than the second one for any $\epsilon \geq 0$. Indeed, the difference is $\frac{250}{3} + \frac{65}{9}\epsilon + \frac{1}{12}\epsilon^2$, and this shows that the UPGMA tree could be arbitrarily bad.

# 3 The geometry of projections

In the preceding section we showed that UPGMA performs an orthogonal projection of $(d(i,j))$ onto a distinguished cone of the complex $\mathcal{F}_n$. It is not immediately clear whether the least squares equidistant tree is obtained by projecting $(d(i,j))$ *orthogonally* onto *some* cone of $\mathcal{F}_n$. Such a tree will be obtained by locating a point on $\mathcal{F}_n$ (a polyhedral complex) that is closest to $(d(i,j))$, and in general, nearest point maps of polyhedral complexes do not have to be given by orthogonal projections onto the *maximal* faces: take for instance the polyhedral complex in $\mathbb{R}^2$ whose maximal faces are the nonnegative $x$-axis together with the nonnegative $y$-axis. For any point with negative coordinates the nearest point is the origin. Although this is obtained by an orthogonal projection onto the origin, these projections are not orthogonal to the maximal faces. In this section, we first show that for $\mathcal{F}_n$ and the Bergman complex $\mathcal{B}_n$ the unexpected happens.

We start with a definition. Given a maximal chain of flats $\mathcal{F}$ of $K_n$ as in Section 2 we let $P_{\mathcal{F}}$ to be the set of points in $\mathbb{R}^{\binom{n}{2}}$ that orthogonally projects

to some point in $C_{\mathcal{F}}$. Since $P_{\mathcal{F}} = C_{\mathcal{F}} + L_{\mathcal{F}}^{\perp}$ where $L_{\mathcal{F}}$ is the smallest subspace containing $C_{\mathcal{F}}$, it is clear that $P_{\mathcal{F}}$ is also a polyhedral cone. We call this cone the *projection cone* of $C_{\mathcal{F}}$.

**Theorem 3.1.** *The projection cone $P_{\mathcal{F}}$ is the full-dimensional cone defined by the $n-2$ inequalities*

$$\frac{1}{|F_k \setminus F_{k-1}|} \sum_{(i,j)\in F_k\setminus F_{k-1}} x(i,j) \;\leq\; \frac{1}{|F_{k+1} \setminus F_k|} \sum_{(i,j)\in F_{k+1}\setminus F_k} x(i,j)$$

*where $k = 1, \ldots, n-2$. The common refinement of $P_{\mathcal{F}}$ over all $\mathcal{F}$ is a complete polyhedral fan.*

*Proof.* Let $K_{\mathcal{F}}$ be the cone defined by the above inequalities. The proof of Proposition 2.3 implies that any point in $K_{\mathcal{F}}$ projects to a point in $C_{\mathcal{F}}$: one should only note that if $(x(i,j))$ satisfies the inequalities then $(x(i,j)) + (p(i,j))$ also satisfies them for any $(p(i,j))$ in $L_{\mathcal{F}}^{\perp}$ since vectors in $L_{\mathcal{F}}^{\perp}$ do not change the averages which are on both sides of these inequalities. Conversely, any point in $P_{\mathcal{F}}$ is of the form $(y(i,j)) + (p(i,j))$ where $(y(i,j)) \in C_{\mathcal{F}}$ which trivially satisfies these inequalities. The intersection of any collection of $P_{\mathcal{F}}$ is a nonempty cone since the intersection of *all* $P_{\mathcal{F}}$ contains the line generated by $(1,1,\ldots,1)$ (in fact, it is equal to this line). Moreover, Proposition 2.3 implies that every point in $\mathbb{R}^{\binom{n}{2}}$ is in *some* $P_{UPGMA}$. This shows that the common refinement of $P_{\mathcal{F}}$ is a complete polyhedral fan. □

At the end of this section we will look more carefully at this polyhedral complex obtained by superimposing all $P_{\mathcal{F}}$. For our main result we need two technical lemmas.

**Lemma 3.2.** *Suppose $\mathcal{F}^1$ and $\mathcal{F}^2$ are two distinct maximal chains of flats of $K_n$. Then the interior of $P_{\mathcal{F}^1}$ and the cone $C_{\mathcal{F}^2}$ are disjoint.*

*Proof.* Suppose $\mathcal{F}^j = \{\emptyset = F_0^j \subset F_1^j \subset \cdots \subset F_{n-2}^j \subset F_{n-1}^j = \binom{[n]}{2}\}$ for $j = 1, 2$. Note that the relative interior of $P_{\mathcal{F}^1}$ is defined by the inequalities defining $P_{\mathcal{F}^1}$ except that $\leq$ are replaced by $<$. We suppose that the intersection of the interior of $P_{\mathcal{F}^1}$ and the cone $C_{\mathcal{F}^2}$ is not empty, and we will reach a contradiction. Assume that $F_p^1 = F_p^2$ for $p < q$ and $F_q^1 \neq F_q^2$. Let $(x(i,j))$ be a point in this nonempty intersection, and let $(y(i,j))$ be the projection of this point onto $C_{\mathcal{F}^1}$. Let $(s,t)$ be an edge in $F_q^1 \setminus F_{q-1}^1$. Then we know that $y(i,j) = a$ for all $(i,j) \in F_q^1 \setminus F_{q-1}^1$ and therefore $y(s,t) = a$. The edge $(s,t)$ is in $F_r^2 \setminus F_{r-1}^2$ where $r > q$ since otherwise $F_q^1 = F_q^2$. Since $F_r^2$ is a flat containing $F_{q-1}^2 = F_{q-1}^1$ the general theory of matroids implies that $F_r^2 \setminus F_{r-1}^2$

contains $F^1_q \setminus F^1_{q-1}$. Because $(x(i,j))$ is in $C_{\mathcal{F}^2}$ we conclude that $x(i,j) = b$ for all $(i,j) \in F^2_r \setminus F^2_{r-1}$ and therefore $x(i,j) = b$ for all $(i,j) \in F^1_q \setminus F^1_{q-1}$. The orthogonal projection onto $C_{\mathcal{F}^1}$ keeps the average of these $x(i,j)$ constant. In other words, $a = b$ and $x(i,j) = y(i,j)$ for $(i,j) \in F^1_q \setminus F^1_{q-1}$. Now let $(u,v)$ be an edge in $F^1_{q+1} \setminus F^1_q$. Again we know that $y(i,j) = c > a$ for all $(i,j) \in F^1_{q+1} \setminus F^1_q$, including $y(u,v) = c$. We will show that $(u,v)$ is in $F^2_z \setminus F^2_{z-1}$ where $z > r$. Suppose not. Then $F^2_r \setminus F^2_{q-1}$ contains $F^1_{q+1} \setminus F^1_{q-1}$, and this implies that $x(i,j) = b_{i,j} \leq a$ for all $(i,j) \in F^1_{q+1} \setminus F^1_{q-1}$. But then the orthogonal projection argument implies that $y(i,j) = c \leq a$ for $(i,j) \in F^1_{q+1} \setminus F^1_q$. This is a contradiction and we conclude that $z > r$. The above chain of arguments can be applied to all $F^1_k \setminus F^1_{k-1}$ for $k = q, \ldots, n-1$ to produce a chain $F^2_{r_q} \subset F^2_{r_{q+1}} \subset \cdots \subset F^2_{r_{n-1}}$ where $q < r_q < r_{q+1} < \cdots < r_{n-1} \leq n-1$ (we have constructed the first two members of this chain, namely $r_q = r$ and $r_{q+1} = z$). However, this is a contradiction since there are only $n - 1 - q$ distinct integers bigger than $q$ and at most $n-1$. □

**Lemma 3.3.** *Suppose $\mathcal{F}^1$ and $\mathcal{F}^2$ are two distinct maximal chains of flats in $K_n$. If $P_{\mathcal{F}^1} \cap C_{\mathcal{F}^2}$ is nonempty, then this intersection is contained in $C_{\mathcal{F}^1} \cap C_{\mathcal{F}^2}$.*

*Proof.* This proof invokes similar ideas as in the proof of Lemma 3.2. Suppose $\mathcal{F}^j = \{\emptyset = F^j_0 \subset F^j_1 \subset \cdots \subset F^j_{n-2} \subset F^j_{n-1} = \binom{[n]}{2}\}$ for $j = 1,2$. Assume that $F^1_p = F^2_p$ for $p < q$ and $F^1_q \neq F^2_q$. Let $(x(i,j))$ be a point in $P_{\mathcal{F}^1} \cap C_{\mathcal{F}^2}$, and let $(y(i,j))$ be the projection of this point onto $C_{\mathcal{F}^1}$. We will show that $x(i,j) = y(i,j)$ for all $(i,j)$. By our assumption this is true for all $(i,j) \in F^1_{q-1} = F^2_{q-1}$. Let $(s,t)$ be an edge in $F^1_q \setminus F^1_{q-1}$. Then we know that $y(i,j) = a$ for all $(i,j) \in F^1_q \setminus F^1_{q-1}$ and therefore $y(s,t) = a$. The edge $(s,t)$ is in $F^2_r \setminus F^2_{r-1}$ where $r > q$ since otherwise $F^1_q = F^2_q$. Since $F^2_r$ is a flat containing $F^2_{q-1} = F^1_{q-1}$ we conclude that $F^2_r \setminus F^2_{r-1}$ contains $F^1_q \setminus F^1_{q-1}$. Because $(x(i,j))$ is in $C_{\mathcal{F}^2}$ we have $x(i,j) = b$ for all $(i,j) \in F^2_r \setminus F^2_{r-1}$ and therefore $x(i,j) = b$ for all $(i,j) \in F^1_q \setminus F^1_{q-1}$. The orthogonal projection onto $C_{\mathcal{F}^1}$ keeps the average of these $x(i,j)$ constant. In other words, $a = b$ and $x(i,j) = y(i,j)$ for $(i,j) \in F^1_q \setminus F^1_{q-1}$. Now let $(u,v)$ be an edge in $F^1_{q+1} \setminus F^1_q$. Now we know that $y(i,j) = c \geq a$ for all $(i,j) \in F^1_{q+1} \setminus F^1_q$, including $y(u,v) = c$. Furthermore $(u,v)$ is in $F^2_z \setminus F^1_{z-1}$ where $z > q-1$. If $z \leq r$ then $F^1_{q+1} \setminus F^1_{q-1}$ is contained in $F^2_r$, and therefore $x(i,j) = b_{i,j} \leq a$ for all $(i,j) \in F^1_{q+1} \setminus F^1_q$. If $x(i,j) < a$ for any of these edges, then the average of $x(i,j)$ in this set is strictly less than $a$. But this average is equal to the average of $y(i,j)$ for $(i,j) \in F^1_{q+1} \setminus F^1_q$, and we get a contradiction since this implies $c < a$. Therefore, if $z \leq r$ then $a = c$ and $x(i,j) = y(i,j)$ for all $(i,j)$ in $F^1_{q+1} \setminus F^1_q$. If $z > r$, then $F^2_z \setminus F^2_{z-1}$ contains $F^1_{q+1} \setminus F^1_q$. Therefore $x(i,j) = b$

for all $(i,j) \in F^1_{q+1} \setminus F^1_q$, and the average of these $x(i,j)$ is $b$. But $b = c$ since the average of $x(i,j)$ and $y(i,j)$ is constant for $(i,j) \in F^1_{q+1} \setminus F^1_q$. But this implies $x(i,j) = y(i,j)$ for edges in this set as well. Now we can repeat the same argument for the rest of $F^1_k \setminus F^1_{k-1}$.

□

**Theorem 3.4.** *Let $\mathcal{P}_d$ be the set of projection cones containing the data point $(d(i,j))$. Then the best least squares equidistant tree corresponds to a point in $C_{\mathcal{F}}$ for some $P_{\mathcal{F}} \in \mathcal{P}_d$.*

*Proof.* Let $x = (x(i,j))$ be the point corresponding to the best least square equidistant tree, and let $C$ be the cone of $\mathcal{F}_n$ where $x \in C$. We let $P$ be the projection cone of $C$. If the line segment $\overline{x-d}$ is orthogonal to $C$, then $P \in \mathcal{P}_d$ and we are done. If not, we show that $x$ is on the boundary of $C$ (and hence $P$). Suppose that $x$ is in the relative interior of $C$, and hence in the interior of $P$. If $\overline{x-d}$ is entirely contained in $P$, then it must be perpendicular to $C$ and this would imply that $P \in \mathcal{P}_d$. Hence let $y = (y(i,j))$ be the first point on $\overline{x-d}$ which intersects $P$. Clearly, $y$ must be on the boundary of $P$. If we let $y'$ be the orthogonal projection of $y$ onto $C$, then we conclude that $||y'-d|| < ||y-d||+||y'-y|| < ||y-d||+||x-y|| = ||x-d||$, and this is a contradiction. Hence $x$ is on the boundary of $C$ and $P$. Now let $\mathcal{P}_x$ be the projection cones containing $x$. Since $x$ is on the boundary of $P \in \mathcal{P}_x$, and by Lemma 3.2, none of the projection cones in $\mathcal{P}_x$ can contain $x$ in their interiors. If we let $\mathcal{P}_x = \{P_{\mathcal{F}_1}, \dots, P_{\mathcal{F}_k}\}$, then by Lemma 3.3 $x$ is contained in (the boundaries of) $C_{\mathcal{F}_1}, \dots, C_{\mathcal{F}_k}$. Now only two things can happen. Either $\overline{x-d}$ is entirely contained in one of $P_{\mathcal{F}_i}$ where $i = 1, \dots, k$, in which case this cone also belongs to $\mathcal{P}_d$, and we are done, or otherwise for each $P_{\mathcal{F}_i}$ there is a first point $y_i$ on $\overline{x-d}$ intersecting $P_{\mathcal{F}_i}$. Repeating the above argument we can conclude that $y_i = x$ for all $i$. This means that for every point $y$ on $\overline{x-d}$ $\mathcal{P}_y$ is disjoint from $\mathcal{P}_x$. But since the projection cones are closed cones this is a contradiction, unless $x = d$. □

In the light of Theorem 3.4 we introduce a graph $\mathcal{G}_{n,d}$ associated to each data point $d = (d(i,j))$ in $\mathbb{R}^{\binom{n}{2}}$. The vertices of this graph are $C_{\mathcal{F}}$ where $P_{\mathcal{F}} \in \mathcal{P}_d$, and there is an edge between two vertices $C_{\mathcal{F}^1}$ and $C_{\mathcal{F}^2}$ if these two cones in $\mathcal{F}_n$ share a facet.

**Proposition 3.5.** *The graph $\mathcal{G}_{3,d}$ is either $K_1$, $K_2$ or $K_3$, and when $n \geq 4$, $\mathcal{G}_{n,d}$ could have more than one component.*

*Proof.* At most two out of the three inequalities $d_{12} \leq (d_{13} + d_{23})/2$, $d_{13} \leq (d_{12} + d_{23})/2$, and $d_{23} \leq (d_{12} + d_{13})/2$ hold unless $d_{12} = d_{13} = d_{23}$. In the

latter case $\mathcal{G}_d = K_3$, and otherwise $\mathcal{G}_d = K_j$ if $j = 1, 2$ of the inequalities are satisfied. We use the following data to illustrate that $\mathcal{G}_{4,d}$ can be disconnected:

$$(d(1,2), d(1,3), d(1,4), d(2,3), d(2,4), d(3,4)) \; = \; (1,2,3,2,7,3).$$

The set $\mathcal{P}_d$ consists of four cones, and hence there are four trees one can obtain. The component of the UPGMA tree has a total of two trees, and there are two more components where each component is just one tree. $\square$

We finish this section by studying the polyhedral complex we defined in Theorem 3.1, namely the common refinement of the projection cones $P_{\mathcal{F}}$ for each maximal cell $C_{\mathcal{F}}$ in the Bergman complex $\mathcal{B}_n$. We denote this complex by $\mathcal{Q}_n$. Note that $\mathcal{Q}_n$ is full dimensional complex in $\mathbb{R}^{\binom{n}{2}}$, and the interior of a full dimensional cell in $\mathcal{Q}_n$ consists of those data vectors which project to the same set of $C_{\mathcal{F}}$.

**Example 3.6.** When $n = 3$ the complex $\mathcal{Q}_3$ is easy to describe. There are total of six maximal cells which are of two different types. The first type consists of those vectors which project to exactly one of the three $C_{\mathcal{F}}$. The second type consists of those vectors which project to exactly two $C_{\mathcal{F}}$.

**Example 3.7.** When $n = 4$ at most six distinct projection cones could have an intersection that gives a maximal cell in $\mathcal{Q}_4$ as we checked with a short MAPLE program. There are a total of 166 such cells, but they come in ten different orbits with respect to the action of $S_4$. The following table lists a representative of each orbit. Since the projection cones are indexed by binary trees on four leaves, we just list these trees.

| orbit representative | orbit size |
|---|---|
| (((1,2),3),4) (((1,2),4),3) (((1,3),2),4) (((1,3),4),2) (((1,4),2),3) (((1,4),3),2) | 4 |
| (((1,2),3),4) (((1,2),4),3) (((1,3),2),4) (((1,3),4),2) (((1,4),2),3) ((1,4),(2,3)) | 24 |
| (((1,2),3),4) (((1,2),4),3) (((1,3),2),4) (((1,4),2),3) ((1,3),(2,4)) ((1,4),(2,3)) | 12 |
| (((1,2),3),4) (((1,2),4),3) (((1,3),2),4) (((1,4),3),2) (((2,4),1),3) ((1,3),(2,4)) | 24 |
| (((1,2),3),4) (((1,2),4),3) (((1,3),2),4) (((2,3),4),1) (((2,4),3),1) ((1,3),(2,4)) | 24 |
| (((1,2),3),4) (((1,2),4),3) (((1,3),2),4) (((2,4),1),3) ((1,3),(2,4)) ((1,4),(2,3)) | 12 |
| (((1,2),3),4) (((1,3),2),4) (((1,4),2),3) (((2,4),1),3) ((1,3),(2,4)) ((1,4),(2,3)) | 24 |
| (((1,2),3),4) (((1,3),2),4) (((2,4),1),3) (((3,4),1),2) ((1,2),(3,4)) ((1,3),(2,4)) | 12 |
| (((1,2),3),4) (((1,3),2),4) (((2,4),1),3) (((3,4),2),1) ((1,2),(3,4)) ((1,3),(2,4)) | 24 |
| (((1,2),3),4) (((1,3),2),4) (((2,4),3),1) (((3,4),2),1) ((1,2),(3,4)) ((1,3),(2,4)) | 6 |

**Theorem 3.8.** *There is a maximal cell in $\mathcal{Q}_n$ which is the intersection of at least $(n-1)!$ projection cones; i.e., there are data vectors in $\mathbb{R}^{\binom{n}{2}}$ which orthogonally project onto at least $(n-1)!$ (non-degenerate) equidistant trees.*

*Proof.* Let $a < b$ two real numbers and let $x(i,j) \in \mathbb{R}^{\binom{n}{2}}$ be the data vector where $x(1,j) = a$ for $j = 2,\dots,n$ and $x(i,j) = b$ for all other components. We claim that this vector is in the interior of the intersection of $(n-1)!$ projection cones corresponding to the comb trees of the form $(\cdots((1,a_2),a_3)\cdots),a_n)$ where $a_2,a_3,\dots,a_n$ run through all permutations of $\{2,\dots,n\}$. For any one of these trees our data vector is in the interior of the corresponding projection cone if and only if

$$a < \frac{a+b}{2} < \frac{a+2b}{3} < \frac{a+3b}{4} < \cdots < \frac{a+(n-2)b}{n-1}.$$

The above inequalities hold for the choice of $a$ and $b$ we made. This proves the theorem. □

This theorem asserts that there are maximal cells in $\mathcal{Q}_n$ that are intersections of *at least* $(n-1)!$ projection cones. We believe that the number of such cones cannot exceed $(n-1)!$, though we do not have a proof.

**Conjecture 3.9.** *The maximal cells in $\mathcal{Q}_n$ are obtained as the intersection of at most $(n-1)!$ projection cones.*

# 4 Extended UPGMA and Branch-and-Bound

In view of the results in Section 3 we propose two algorithms. The first one is an extension of the usual UPGMA which searches the component of the graph $\mathcal{G}_{n,d}$ to which the UPGMA tree belongs to. Even when this component is large this extended UPGMA algorithm performs well and finds the best tree in this component. The drawback of this algorithm is that it may not produce the best tree. Our second algorithm is an exact algorithm which produces the best equidistant tree with a branch and bound approach on the space of maximal chains of the lattice of contractions of $K_n$. We will present this as a shortest path algorithm on the Hasse diagram of this lattice. Recall that this lattice is isomorphic to the partition lattice $\Pi_n$ where maximal chains are in bijection with the maximal cones in $\mathcal{F}_n$.

**Algorithm 4.1.** Extended UPGMA
**Input** : Complete graph $K_n$ with edge weights $d(i,j)$.
**Output**: An equidistant tree $T$ with leaves $X = \{1,\dots,n\}$ and $x(i,j)$ for each $i,j \in X$.

Using Algorithm 1.1 find the UPGMA tree $T_{UPGMA}$ and the corresponding cone $\mathcal{C}_{UPGMA}$ in the Bergman compex $\mathcal{B}_n$.
Let $\texttt{Visited} := \{T_{UPGMA}\}$, $\texttt{Active} := \{T_{UPGMA}\}$, and $T_{best} := T_{UPGMA}$.
**while** $\texttt{Active} \neq \emptyset$ **do**
  Let $T \in \texttt{Active}$ and $\texttt{Active} := \texttt{Active} \setminus \{T\}$.
  **for** each $\mathcal{C}_{T'} \in \mathcal{B}_n$ which shares a facet with $\mathcal{C}_T$ **do**
    **if** $\mathcal{C}_{T'} \in \mathcal{P}_d$ and $T' \notin \texttt{Visited}$ **then**
    $\texttt{Active} := \texttt{Active} \cup \{T'\}$ and $\texttt{Visited} := \texttt{Visited} \cup \{T'\}$
    If $\sum(d(i,j) - x_{T'}(i,j))^2 \quad < \quad \sum(d(i,j) - x_{T_{best}}(i,j))^2$ then $T_{best} := T'$.
    **end if**
  **end for**
**end while**

Output $T_{best}$ and $x_{T_{best}}(i,j)$ $1 \leq i < j \leq n$.

A few remarks about Algorithm 4.1 are in order: This algorithm searches the component of $\mathcal{G}_{n,d}$ to which $\mathcal{C}_{UPGMA}$ belongs, and it outputs the best equidistant tree in this component. If $\mathcal{G}_{n,d}$ consists of a single component then the algorithm's output is the optimal tree. The search depends on the following characterization of Ardila and Klivans [2] when $\mathcal{C}_{\mathcal{F}^1}$ and $\mathcal{C}_{\mathcal{F}^2}$ share a facet in $\mathcal{B}_n$. Finally, checking whether a cone $\mathcal{C}_T$ belongs to $\mathcal{P}_d$ is trivial by Theorem 3.1.

**Proposition 4.2.** *Two maximal cones $\mathcal{C}_{\mathcal{F}^1}$ and $\mathcal{C}_{\mathcal{F}^2}$ share a facet in $\mathcal{B}_n$ if and only if there exists $0 < j < n-1$ such that $F_i^1 = F_i^2$ for all $i = 0, \dots, n-1$ except $F_j^1 \neq F_j^2$ and $(F_j^1 \setminus F_{j-1}^1) \cap (F_j^2 \setminus F_{j-1}^2) \neq \emptyset$.*

Our exact algorithm is a modified shortest path algorithm performed on the Hasse diagram of the partition lattice $\Pi_n$. We first introduce some notation for this algorithm. We will represent this Hasse diagram as a directed graph where the nodes are labeled by flats of $K_n$, and the edges are directed from the minimum element (corresponding to the empty flat) to the top element (corresponding to the flat $[n] = \{1, \dots, n\}$). For each node (flat) $F$ we will keep track of *incoming* edges $I_F$ and *outgoing* edges $O_F$. Each edge is directed from a flat $F_i$ to a flat $F_{i+1}$ of next rank such that $F_i \subset F_{i+1}$. Each such edge $e$ will have two associated numbers, $x(e)$ and $\ell(e)$, which will be defined throughout the algorithm using the given data $(d(i,j))$.

**Algorithm 4.3.** Exact least squares
**Input** : Complete graph $K_n$ with edge weights $d(i,j)$.
**Output**: The best least square equidistant tree $T$ with leaves $X = \{1,\dots,n\}$ and $x(i,j)$ for each $i,j \in X$.

Set $\texttt{Active}_0 := \{\emptyset\}$, $I_\emptyset := \{g\}$, $x(g) := -\infty$, and $\ell(g) := 0$.
Set $V := \texttt{Active}_0$ and $A := \{\}$.
**for** $k = 0, 1, \dots, n-1$ **do**
$\texttt{Active}_{k+1} := \{\}$.
  **while** $\texttt{Active}_k \neq \emptyset$ **do**
    Let $F \in \texttt{Active}_k$ and $\texttt{Active}_k := \texttt{Active}_k \setminus \{F\}$.
    **for** each $e = (F, F') \in O_F$ **do**
      Set $x(e) := \frac{1}{|F' \setminus F|} \sum_{(i,j) \in F' \setminus F} d(i,j)$ and $E := \{f \in I_F \,:\, x(e) \geq x(f)\}$.
      **if** $E = \emptyset$ **then** $x(e) := +\infty$ **else** $h := \mathrm{argmin}\{\ell(f) \,:\, f \in E\}$ **end if**
      $\ell(e) = \ell(h) + w(e)$ where $w(e) = \sum_{(i,j) \in F' \setminus F} (x(e) - d(i,j))^2$
      **if** $x(e) < +\infty$ **then**
        $\texttt{Active}_{k+1} := \texttt{Active}_{k+1} \cup \{F'\}$ and $A := A \cup \{e\}$
      **end if**
    **end for**
  **end while**
$V := V \cup \texttt{Active}_{k+1}$.
**end for**

Find the shortest path $P$ from $\emptyset$ to $[n]$ in the graph $G = (V, A)$ with edge weights $w(e)$ for $e \in A$.

Output the tree $T$ corresponding to $P$ and $x_T(i,j)$ $1 \leq i < j \leq n$.

*Proof of Correctness*: Each path $P$ in $G$ from the empty flat to the full flat corresponds to a flag $\mathcal{F}$ and hence a cone $\mathcal{C}_\mathcal{F}$. By the construction of $G$, the $x(e)$ for the edges $e$ on such a path give a point in $\mathcal{C}_\mathcal{F}$, and this point is the orthogonal projection of $(d(i,j))$ onto $\mathcal{C}_\mathcal{F}$. In other words, a path $P$ in $G$ corresponds to a cone $\mathcal{C}_\mathcal{F} \in \mathcal{P}_d$. Since $\sum_{e \in P} w(e)$ is the Euclidean distance from the data point to the projection in $\mathcal{C}_\mathcal{F}$, Theorem 3.4 implies the correctness of the algorithm if for each $\mathcal{C}_\mathcal{F} \in \mathcal{P}_d$ there is a path $P$ in $G$ from $\emptyset$ to $[n]$. We show by induction on $i$ that $G$ contains the edges $e_i = (F_{i-1}, F_i)$ corresponding to the flag $\mathcal{F}$. It is trivial to check that $e_1 = (\emptyset, F_1)$ is in $G$. Moreover $x(e_1) = d(i,j)$ where $F_1 = \{(i,j)\}$. We assume that $e_k$ for $k \leq i-1$ are in $G$. Note that each $e_k$ is added to $G$ during the $k$th pass of the outermost for loop. Now $x(e_i) = \frac{1}{|F_i \setminus F_{i-1}|} \sum_{(i,j) \in F_i \setminus F_{i-1}} d(i,j)$, and because $\mathcal{C}_\mathcal{F} \in \mathcal{P}_d$ we

conclude that $x(e_i) \geq x(e_{i-1})$. Since $e_{i-1} \in I_{F_{i-1}}$ the set $E$ during the pass of the innermost for loop corresponding to $e_i$ is nonempty and hence $x(e_i)$ stays finite. This means $e_i$ is added to $G$. □

For the purposes of the exposition of Algorithm 4.3 we have chosen to first construct the graph $G$ in the algorithm and then solve the shortest path problem on this graph. In fact one can skip the construction of $G$ if one adds a pointer to each edge $e$ that points to the corresponding edge $h$ in the algorithm. With these pointers one can reconstruct the shortest path and hence the best equidistant tree $T$ at the end of the algorithm. Note that this algorithm is a branch and bound algorithm on the space of all maximal chains in $\Pi_n$ starting from the empty flat: whenever $x(e) = +\infty$ for some $e$ being considered then all such maximal chains containing $e$ are pruned from the branch and bound tree. The branching step is realized when we extend a chain terminating at the node labeled $F$ by adding $e = (F, F') \in O_F$ for all such edges where $x(e) < +\infty$.

# 5 A biology example

How does the least squares approach compare to Bayesian and maximum likelihood methods in practise? We compared the different methods on a problem in evolution for which some of the data shows clock-like behavior. Murphy et al. (2001) have studied the timing and sequence of appearence of the mammalian orders using a large DNA database that includes 42 placental mammals from all orders, plus two marsupials as the outgroup. The model of sequence evolution employed by Murphy et al. (and by us) was the general-time-reversible+$\Gamma$+invariants model. Bayesian and maximum likelihood methods converged on the same combinatorial type of tree (Murphy et al., 2001). Distances estimated during likelihood fitting using this model do not satisfy the clock hypothesis over the complete dataset; however a subset of eleven species do show clock-like substitution rates (Murphy et al.,2001, supplemental material). Distances from ten of these taxa were analyzed here using the exact least squares algorithm. The main conclusions of Murphy et al. on the branching sequence are supported by the best least squares tree: first the Afrotherians, then the Xenartharns and finally the Boreoeutherians separate from their placental ancestors. The only difference between the ten taxa least squares and maximum likelihood trees is the position of the dolphin. Murphy et al. scaled their tree to obtain dates using 50 mya for the cat/canid divergence. Scaling the best least squares tree in the

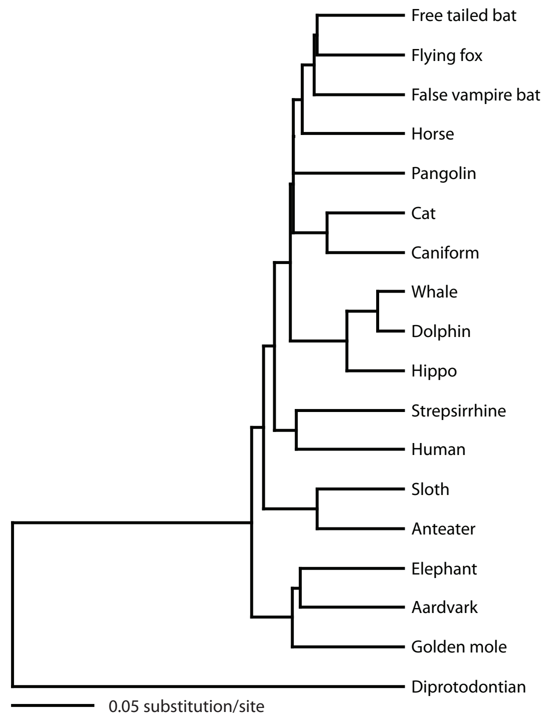


Figure 3: Example of mammalian phylogeny obtained by extended UPGMA

same way gives 107 and 101 million years ago for the bifurcations producing the Afrotherians and Xenarthrans, respectively. The corresponding values reported by Murphy et al., 2001, are 103 and 95 million years ago. Hence the agreement between the least squares and Bayesian or likelihood methods is quite good.

Visual inspection of the complete phylogram from the 44 taxa dataset suggested that others were nearly contemporaneous with those in the eleven taxa subset. For a sequence of datasets ranging from eleven to nineteen species, three trees were identified: we found the maximum likelihood tree, the maximum likelihood equidistant tree, and the best least squares equidistant tree. Species added to the eleven taxa subset were the roussette fruit bat, anteater, whale, hippopotamus, aardvark, human, horse and sciurid. The inexact form of the least squares equidistant tree algorithm was used

on these datasets with more than ten taxa. For the trees with twelve up to eighteen taxa the number of possible least squares trees was either one or two, with the best least squares tree being the UPGMA tree in each case. The eighteen taxa dataset had two possible trees, the better was the non-UPGMA tree (Figure 3). When the sciurid data was then added to create a dataset with nineteen taxa, the number of possible trees jumped to six.

The number of possible trees for datasets up to eighteen taxa is small compared to the conjectured $(n-1)!$ upper limit of trees, indicating that the distances were close to clock-like. Hence the corresponding equidistant trees should be good approximations to the phylogeny. As distances that deviate more from clock-like behavior are added, the number of possible trees increases and the equidistant tree gives a poorer account of the phylogeny.

When two least squares equidistant trees were possible for a given dataset, the oldest bifurcations were conserved between the two, with the differences appearing in more recent branchings. This observation is expected. For a given internal node the distance to a leaf is one-half the average of all path lengths between pairs of leaves that pass through that node. More paths pass through the older nodes, so their ages are estimated more accurately. Unless old bifurcations occur very close to each other, they will be more stable in the set of possible trees. The best least squares trees with up to eighteen taxa all confirmed the branching order of the Afrotherians, Xenarthrans and Boreoeutherians observed by Murphy et al., 2001.

There was one persistent difference between the likelihood and least squares approaches: the equidistant least squares trees placed the cetartiodactyls as an outgroup to the carnivores, bats and pangolin, whereas the maximum likelihood trees put the bats as an outgroup. It is a bit surprising, since the likelihood and distance methods are both consistent in the statistical sense, and therefore expected to converge on the same, correct, tree (Felsenstein, 2004). The dataset contains 17028 characters, but perhaps more data is needed, or a different sample of sequences, to obtain convergence on one tree.

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